Bentazone

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 304 °C

Global applicability domain: Outside

Local applicability domain index: 2.32e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found
2-Nitrobenzamide
Measured: 317
Predicted: 310

Image not found
3-Nitrobenzamide
Measured: 313
Predicted: 310

Image not found
Diphenylurea
Measured: 262
Predicted: 269

Image not found
Benzoic acid, 2-phenylhydrazide
Measured: 314
Predicted: 306

Image not found
N-Butylbenzenesulfonamide
Measured: 314
Predicted: 286